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This project is focused on the application of a new technique in detecting DNA samples in the frequency range of millimeter to submillimeter wavelengths. This technique is based on the detection of millimeter wave absorption features correspondiing to local vibrational modes of the DNA chains, due to natural lesions induced by broken or stretched (weakened) hydrogen bonds, missing atoms or groups, additional or missing dimers, and substitutional impurities, etc. The samples are in the forms of either thin films or aerosols. In this report we document our experimental findings of the millimeter wave absorption spectra of various DNA biopolymers in the sample form of thin films or aerosols. We have investigated thin film sample of BA, BG, and BT, as well as aerosol samples of BG and BT. We have also studied theoretically the interaction of localized phonon and plasmon modes with electromagnetic radiation, and predicted the absoprtion spectrum theoretically.

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# Millimeter Wave Absorption Measurement on DNA Polymers in Biological Aerosols: Contribution of Localized Phonon and Plasmon Modes

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# Abstract

This project is focused on detecting DNA samples in the frequency range of millimeter to submillimeter wavelengths. Our technique is based on the detection of millimeter wave absorption features corresponding to local vibrational modes of the DNA chains, due to natural lesions induced by broken or stretched (weakened) hydrogen bonds, missing atoms or groups, additional or missing dimers, and substitutional impurities, etc. The samples are prepared in the form of aerosols, with DNA powder of fine particles suspended in innert gas (such as helium). Compared with traditional thin film samples, aerosol affords the added flexibility of varying the particle size and density of particles in the aerosol. With a millimeter wave source capable of continuous sweep of frequencies from 180 GHz to 220 GHz, and high-sensitivity detectors custom-made for the source, several possible characteristic absorption features of DNA samples are uncovered. In connection with the experimental activities of this project, we have also studied the interaction of electromagnetic wave (in the microwave to millimeter wave region) with the localized phonon modes and extended plasmon modes of long-chain DNA polymers. In particular, we calculate the absorption coefficient of the electromagnetic wave by the various modes of the DNA polymers. In this, we first introduce the formulation of normal modes due to both long-range and short-range interactions in the DNA polymer, establishing a way to calculate the eigenmode frequencies and their associated eigenvectors, which are then converted to electrical dipole moments associated with the normal modes. We then consider the electromagnetic wave interaction with DNA polymers in the dipole approximation. From this, we calculate the optical absorption coefficient. We compare our calculations with available experimental data and attempt to interpret the data in light of our calculated results.

# 1 Introduction

It has long been recognized that rapid detection and identification of microorganisms represent pressing needs for various projects in the Department of Defense[1]. Optical techniques such as near-infrared scattering, ultra violet fluorescence, IR absorption, and resonance Raman scattering can be used to detect the presence of biological microorganisms[2–5], but give little specificity as to the exact organism that may be present. However, it is recognized that there are still important advantages to optical techniques. In particular, optical techniques can be used in a standoff mode, where the sample is examined remotely and does not have to be extracted from the environment. This offers many operational advantages for a possible field-type instrument. Thus, there is a high payoff of an optical instrument that satisfies the needs of DoD from an operational point of view. Currently, there is much interest in developing such instruments, although the technical challenges are formidable. Recent advances in understanding the interaction between microwave/millimeter-wave (MMW) radiation and living matters have opened new avenues in detecting and identifying microorganisms. In particular, deoxyribonucleic acid (DNA) is thought to interact with electromagnetic radiation in the MMW region of the spectra, due to the presence of phonon modes and plasmon modes of base pairs along the double helix of the DNA chain[6–9]. Solitons may also be present in the DNA chain. However, as solitary waves are inherently nonlinear, and as such they require significant excitation energies. Phonon modes are primarily mechanical in nature, and travel along the DNA chain at a speed of about 2 $km/s$. The plasmon modes are, essentially, charge density waves and are thought to travel along the DNA chain at a speed of about 36 $km/s$. There is some evidence that the plasmon modes may be overdamped; therefore, they are extremely difficult to observe. On the other hand, the phonon modes are well defined resonances over a wide range of the frequency spectrum (from a few GHz to several THz), and should be readily accessible to experimental observation.

Until recently, the 80 GHz to 1000 GHz region of the electromagnetic spectra have been difficult for spectral observations. Techniques have only recently become available for such spectroscopic studies[10–12]. Recently, there has been proposals for the use of some of the state-of-the-art MMW techniques to observe and identify some of the phonon modes of the DNA

polymers. If successful, this breakthrough may form the basis of a detection system suitable for microorganism field detection. In the frequency range of interest here the spectral features predicted by theoretical studies arise primarily from localized motions, spread over one or more base-pair units. Detailed descriptions will depend on the strength and range of the interactions, such as van der Waals interaction, electronic exchange interactions, Coulombic interactions, and hydrogen bonding. Based on available physical parameter values and reasonable assumptions, a series of resonances are predicted in this spectral region. However, These previous predictions may only serve as a guide, insofar as some of the parameters are not known exactly, and more importantly, the theories are model-dependent and may not be completely accurate. For example, shifted frequencies and changed intensities are to be expected for DNA polymers in different environments (e.g., in water or other solutions, as compared with dry samples). However, it is reasonable to assume that, at or near some of the resonant frequencies predicted (in the frequency region from 80 GHz to 1000 GHZ), some spectral features should be detectable.

It is believed that the distinct features in previous far-IR spectra may be the signature of lesion-induced vibrational modes. When the translational symmetry of the long DNA chain is broken by defects such as broken bonds, missing atoms or groups, additional dimers, substitutional impurities, and the like, vibrations of atoms in the vicinity of the defect lead to distinctive modes which are essentially localized spatially about the defects. This contrasts with the more common sound-like modes of vibration of the long-chain DNA polymers, in which every atom of the chain takes part in the motion. For each separate defect a spectroscopically distinctive characteristic, local-mode frequency exists. The local modes, therefore, provide direct information on the nature of the defect, and can serve as a diagnostic signature of the polymer chain lesion. It is expected that the lines corresponding to local modes will be well-defined, and should be easier to detect. The allowed vibration frequencies associated with the localized defect and the corresponding relative motion of the nearby atoms are of great potential interest for their diagnostic possibilities. Spectroscopic observation of these should provide information on characteristics of particular lesions, and should be related to the irregularities of the DNA polymer structure. The relative intensities of spectral features characteristic of each lesion will be a direct measure of the degree of damage sustained by

the DNA polymer. An analysis of the absorption spectra of known defects/lesions in DNA samples will be a powerful tool for obtaining information about particular inter-atomic interaction and can be used to identify the species in question.

This project is concerned with the experimental investigation of the possibility of detection DNA polymers by millimeter wave absorption spectroscopy, and the theoretical interpretation of the observed MMW absorption spectra of DNA polymers. In particular, we are interested in determining the contribution from the various phonon modes and plasmon modes. This should help in identifying the absorption peaks of the observed spectra. Furthermore, by calculating the various transition matrix element and absorption coefficient, the relative intensities of the spectral lines can be inferred and compared with experiment. Or conversely, Knowledge of the intensities of the observed absorption lines should help in identifying not only the particular modes, but also the spectral weight it carries. In this report, we first present our experimental procedures and results of the millimeter wave absorption spectroscopy of several aerosol samples containing DNA biopolymers. We then describe how the normal modes of the system are calculated. Following that, we describe the theory of interaction of electromagnetic waves with the DNA polymers, and how this interaction excites the various normal modes and leads to features in the absorption spectrum. Our formalism leads naturally to the absorption coefficient of the DNA polymer system. Finally, we carry out typical calculations and compare with experimental data.

# 2 Experimental Investigation of Millimeter Wave Absorption by DNA Polymers

We have carried out preliminary experimental study of the millimeter wave absorption spectrum of various DNA aerosols and thin films. In this study we have employed a simple experimental setup of using a pair of horn-shaped antennas facing each other, with one transmitting and one receiving the millimeter wave signal. The aerosol samples permeate the space between the antennas. In the case of thin film samples, the samples are located midway between the two antennas. Figure 1 is a block diagram of the experimental setup.

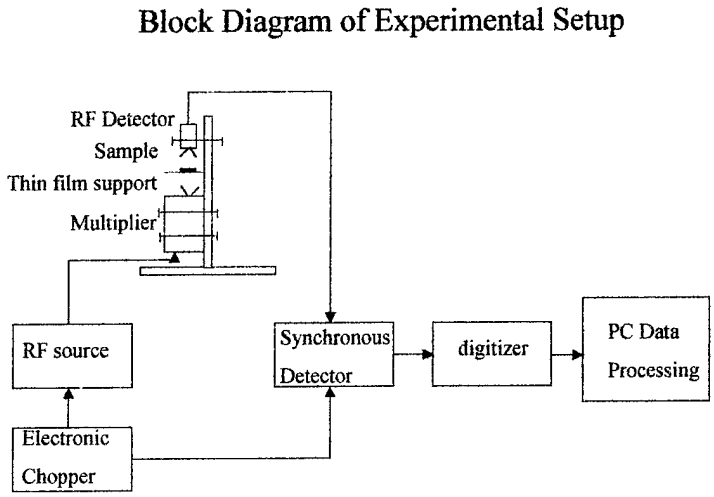


Figure 1: Block diagram of the experimental setup.

The absorption coefficient $\alpha(\nu)$ of the sample as a function of frequency $\nu$ can be determined from the transmission measurements. It can be expressed as

$$\alpha(\nu) = \frac{1}{l} \ln \left( \frac{P_1(\nu)}{P_2(\nu)} \right), \tag{1}$$

where $P_1(\nu)$ is the power measured by the detector without the sample and $P_2(\nu)$ is the power measured by the detector with the sample. $l$ is the path length of the signal through the sample.

In Figures 2-4 we present some of the absorption spectra of various aerosol samples. These include BT, BG, and BA samples.

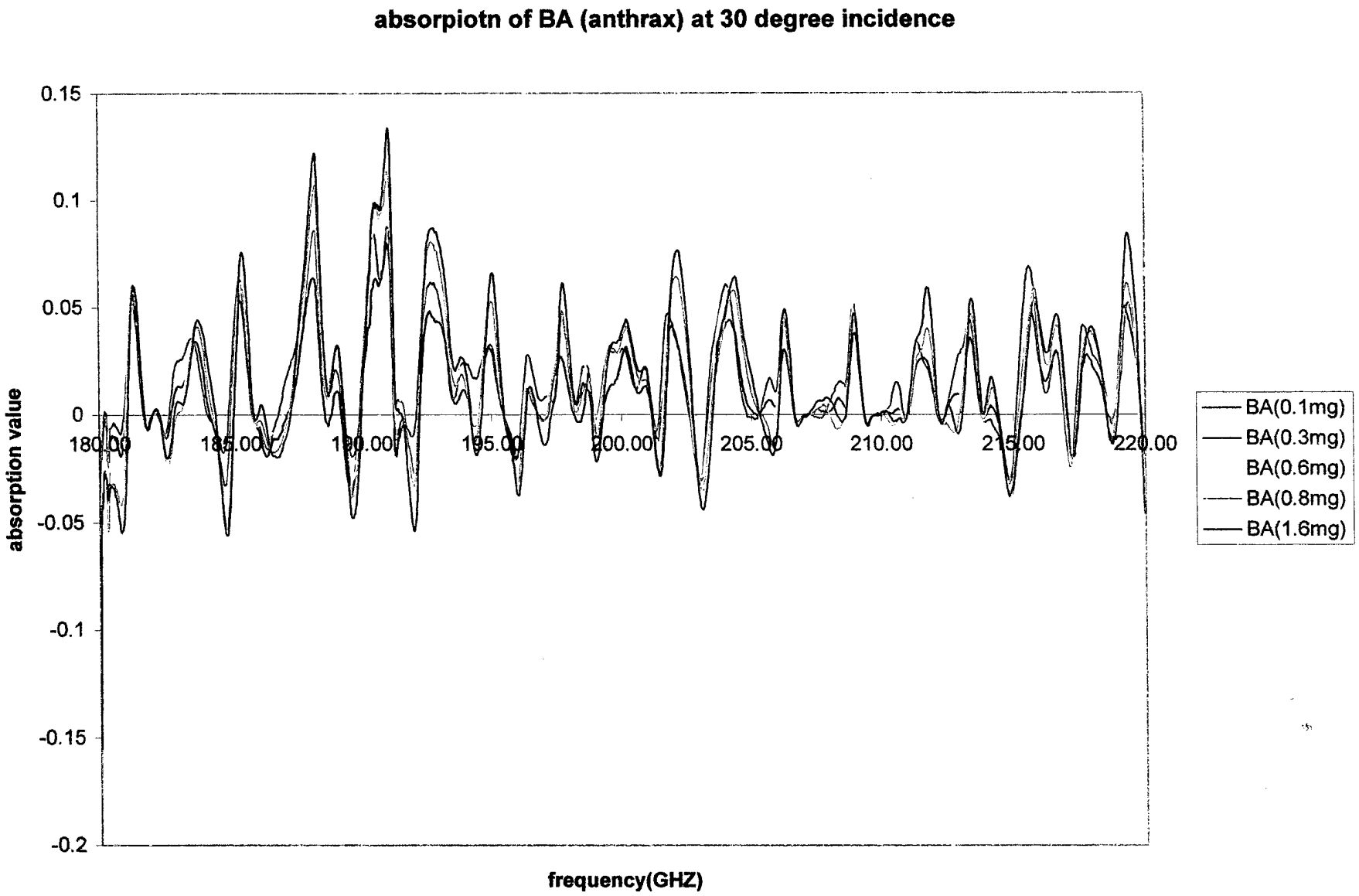


Figure 2: Absorption spectrum of thin film samples of BA (anthrax) at 30 degree incidence for various concentrations.

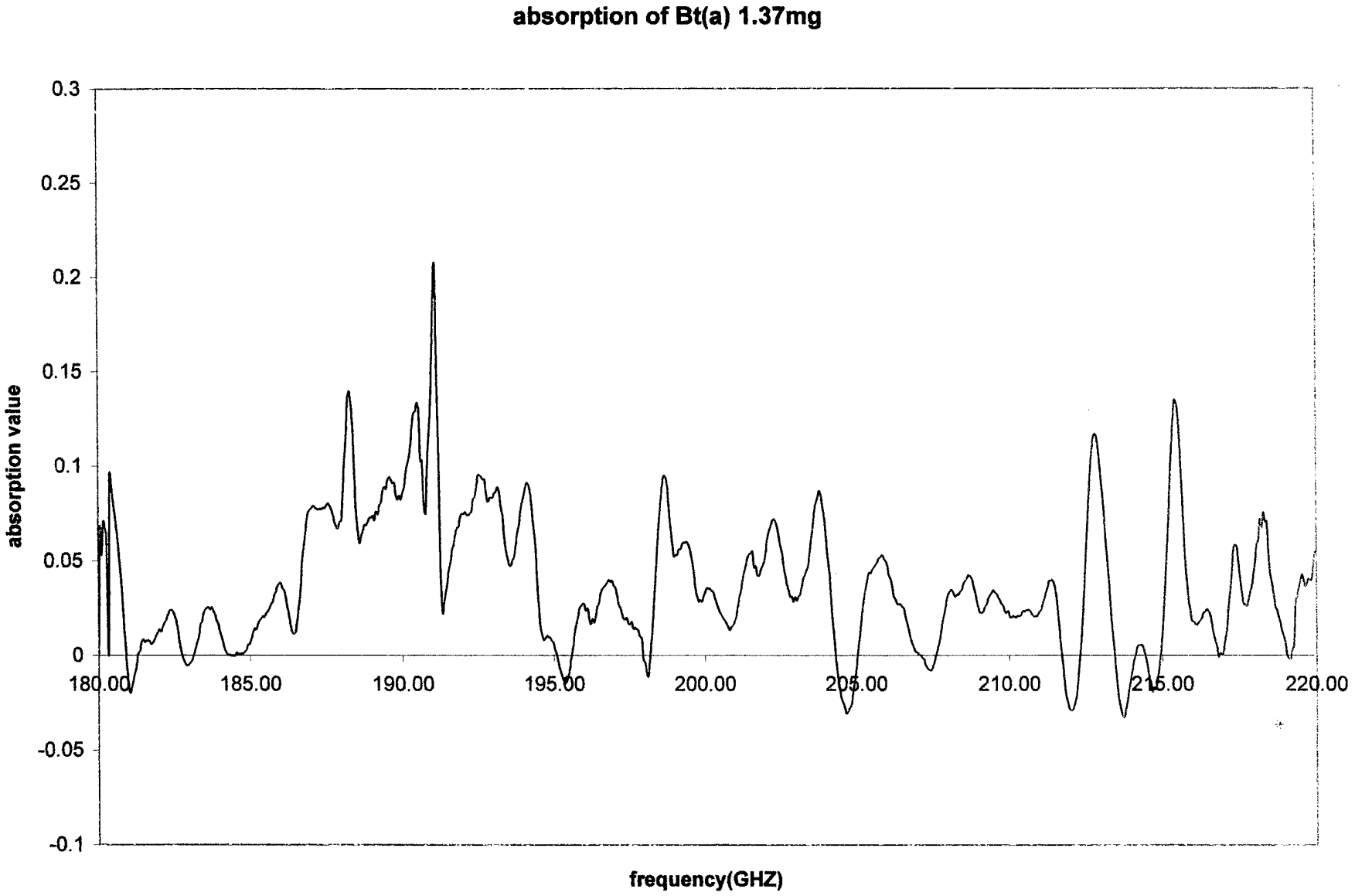


Figure 3: Absorption spectrum of BT aerosol sample.

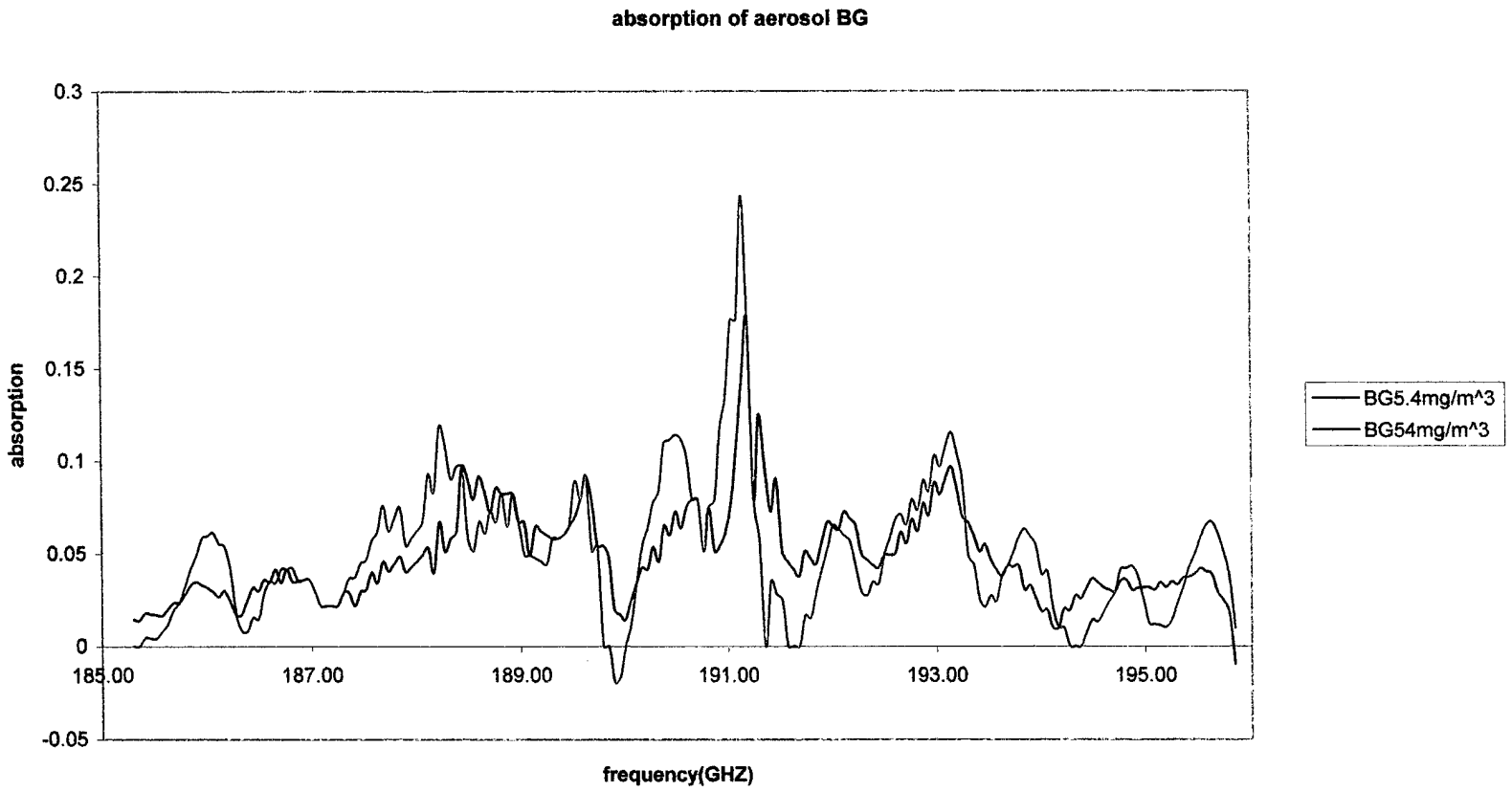


Figure 4: Absorption spectrum of BG aerosol samples for two concentrations.

# 3 Theoretical Study of Millimeter Wave Absorption by DNA Polymers

## 3.1 Normal Modes of a DNA Polymer

In this section we briefly outline the process of calculation of normal modes frequencies and associated eigenvectors for a long chain DNA polymer. We start with the equation of motion for the individual atoms on the chain,

$$m_i \frac{\partial^2 \delta r_i^\alpha}{\partial t^2} = \sum_{j,\beta} F_{i,j}^{\alpha,\beta} \delta r_j^\beta, \tag{2}$$

where $m_i$ is the mass and $\delta r_i^\alpha$ is the $\alpha$th component of the displacement ($\alpha = x, y, z$) of atom $i$ in the unit cell. $F_{,j}^{\alpha,\beta}$ is the force constant matrix for the dry, isolated molecule. Assuming harmonic time dependence of the form $\exp(-i\omega t)$ and using the mass-weighted coordinates $q_i^\alpha = \sqrt{m_i}\delta r_i^\alpha$, Eq. (1) reduces to

$$-\omega^2 q_i^\alpha = \sum_{j,\beta} D_{i,j}^{\alpha,\beta} q_j^\beta, \tag{3}$$

where $D_{i,j}^{\alpha,\beta} = F_{i,j}^{\alpha,\beta}/\sqrt{m_i m_j}$. Thus, the determination of the small-amplitude vibrational behavior of the DNA polymer system involves the setting up and diagonalization of matrix equation

$$\sum_{j,\beta} (D_{i,j}^{\alpha,\beta} - \omega^2 \delta_{i,j}\delta_{\alpha,\beta}) q_j^\beta = 0. \tag{4}$$

Here, the matrix $D$ essentially describes the pair-wise interactions between two atoms in the system. That as many as 40 base pairs of a total of 123 degrees of freedom each contribute (there are 41 atoms in the unit cell), makes this a $5000 \times 5000$ matrix inversion problem, and all 25 million matrix elements have to be dealt with in some fashion or other. Fortunately, for most calculations the periodic translational invariance along the chain can be exploited. For most calculations, one can use the symmetries of a homopolymer model to reduce the algebraic problem to a manageable $123 \times 123$ matrix inversion problem by working in the wavevector space and applying Bloch theorem. However, if the problem at hand lacks symmetry, such as in the cases of localized anomalies, or ends of chains, the full-scale matrix inversion has to be performed.

The most empirical part of this procedure is the determination of the individual elements of the force matrix. In principle, each element requires the sum of more than 60 contributions from the neighboring atom, including both short-range and long-range interactions. One possible simplification may come from the realization of the Coulombic nature of essentially all the forces (long and short-range). Thus, the forces are essentially electrical. As such, they can be described in an effective field approach. The effective electric field is found from treating the partial charges on the atoms as its sources. And the resultant field act on the partially charged atoms to force them into vibrational motion (among other possibilities.) In such a self-consistent fashion, the dynamic behavior of the long-chain DNA polymer can be described. The data on the force matrix elements are known in case of standard structures and compositions. However, for special cases of defect and dislocations, weakened or broken H-bonds, they have to be evaluated separately.

## 3.2 Interaction of Electromagnetic Wave with DNA Polymers

In this section we consider the absorption of electromagnetic wave by a long-chain DNA polymer via its vibrational modes. The absorption is based on the local electromagnetic field present at the macromolecule. The interaction with the field is via an oscillating dipole associated with the vibrational modes. The latter is calculated from the vibrational displacement eigenvectors and a rigid ion model of fixed net charge per atom (also known as the partial charge.) In the case of microwave/millimeter wave interaction with localized vibrational modes, the wavelength of the electromagnetic wave is the order of a few centimeter to about 1 millimeter, which is much larger than the dimension of one base pair of the DNA polymer. In this case the dipole approximation is adequate in describe the interactions. This approximation is still valid even for a number of base pairs comprising a small segment of the biopolymer.

The interaction of the molecule with an oscillating electric field is described by the interaction Hamiltonian (note that in the dipole approximation one treats the electric field of the

electromagnetic wave as spatially homogeneous, $\vec{E}(\vec{x},t) \sim \vec{E}\cos\Omega t$)

$$H_{int} = \sum_{i,m} e_i \delta\vec{r}_{im} \cdot \vec{E}\cos\Omega t, \tag{5}$$

where $e_i$ is the partial charge of the $i$th atom in the $n$th base pair, and $\delta\vec{r}_{im}$ its position as measured from its equilibrium position. We should point out that the above interaction Hamiltonian is rotationally invariant. In our consideration we choose the $z$ axis to be along the helix axis, and the perpendicular $x$ and $y$ axes differently in each cell. Each base pair can be transformed into the next by rotation through the pitch angle $\psi$ (equals 36°) simultaneous translation through a distance $d$ along the helix axis. Thus, the $\delta x_n$ and $\delta y_n$ directions are progressively rotated by $\psi$ in successive base pairs. This choice of coordinate system greatly simplifies the description of atomic motions at the expense of complicating somewhat the description of the external electric field $\vec{E}$. The latter now must be transformed in the following fashion from the laboratory coordinate system to the coordinate system described above:

$$\begin{pmatrix} E'_x \\ E'_y \\ E'_z \end{pmatrix} = \begin{pmatrix} \cos n\psi & \sin n\psi & 0 \\ -\sin n\psi & \cos n\psi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}. \tag{6}$$

Accordingly, the interaction Hamiltonian now takes the form

$$H_{int} = -\sum_{i,m} e_i x_{im}[\cos(n\psi)\hat{x} + \sin(n\psi)\hat{x}] + y_{im}[-\sin(n\psi)\hat{x} + \cos(n\psi)\hat{y} + z_{im}\hat{z}\cdot\vec{E}\cos\Omega t, \tag{7}$$

where $\vec{E}$ is the electric field in the laboratory coordinates.

As before, we introduce the mass-weighted coordinate $\vec{q}_{im} = \delta\vec{x}_{im}/\sqrt{m_i}$. Taking advantage of the rotation-translational invariance along the chain, this can be expanded in the form

$$\vec{q}_{im} = \frac{1}{N}\sum_{\theta,\ell} e^{-im\theta}\vec{q}(\theta,\ell)Q(\theta,\ell), \tag{8}$$

where $\vec{q}_i(\theta,\ell)$ are the relative amplitudes of the motions of the $i$th atom when the polymer vibrates in the $\theta,\ell$ vibrational mode. These amplitudes are properly normalized so that

$$\sum_i \vec{q}^*_i(\theta,\ell)\cdot\vec{q}_i(\theta',\ell') = \delta_{\theta,\theta'}\delta_{\ell,\ell'}. \tag{9}$$

The $Q(\vartheta, \ell)$ are the actual amplitudes of each normal mode which are given in terms of the creation and annihilation operators ($a^{\dagger}_{\vartheta\ell}$ and $a_{\theta\ell}$) as

$$Q(\theta, \ell) = \left(\frac{\hbar}{2\omega_{\theta\ell}}\right)^{1/2} (a_{-\theta\ell} + a^{\dagger}_{\theta\ell}). \tag{10}$$

In terms of the above transformations, the interaction Hamiltonian takes the form

$$\begin{aligned} H_{int} &= -\sum_{in} \frac{e_i}{\sqrt{m_i}} \sum_{\theta,\ell} \\ &[q_{ix}(\theta,\ell)(\cos n\psi E_x + \sin n\psi E_y) + q_{iy}(\theta,\ell)(\cos n\psi E_y - \sin n\psi E_x) + q_{iz}E_z] \\ &\times \left(\frac{\hbar}{2N\omega_{\theta\ell}}\right)^{1/2} e^{-in\theta}(a_{-\theta\ell} + a^{\dagger}_{\theta\ell}) \cos\Omega t. \end{aligned} \tag{11}$$

Actually, the sum over $n$ can be readily carried out, which for an $N$ base-pair system results in the following expression

$$\begin{aligned} H_{int} &= -\sum_{i} \frac{e_i}{\sqrt{m_i}} \sum_{\theta,\ell} \left(\frac{\hbar N}{2\omega_{\theta\ell}}\right)^{1/2} \\ &\times[(q^{(+)}_{i\ell\theta}\Delta_{\theta-\psi} + q^{(-)}_{i\ell\theta}\Delta_{\theta+\psi})E_t + q_{iz}(\theta,\ell)\Delta_\theta E_z] \\ &\times(a_{-\theta\ell} + a^{\dagger}_{\theta\ell}) \cos\Omega t. \end{aligned} \tag{12}$$

Here,

$$q^{(\pm)}_{i\ell\theta} = \frac{q_{ix}(\theta,\ell) \pm iq_{iy}(\theta,\ell)}{2} e^{\pm i\phi},$$

$E_t$ is the transverse component of the electric field, $\phi$ is the angle between the direction of $E_t$ and the $x$ axis, and

$$\Delta_\theta = \frac{\sin(N\theta/2)}{N\sin(\theta/2)}.$$

It is easy to see that for an infinitely long chain ($N \to \infty$), $\Delta_\theta$ approach a Kronecker $\delta$-function. Thus, only the $\theta = 0$ and $\theta = \pm\psi$ terms will contribute. This means that absorption of the incoming electromagnetic radiation can only take place at frequencies in the dispersion curve corresponding to these values of $\theta$, corresponding to distinctive states of polarization of the incident electromagnetic wave. Namely, for $\theta = 0$, it must be polarized along the chain (longitudinal polarization); and for $\theta = \pm\psi$, it must be polarized in the plane perpendicular to the chain (transverse polarization). On the other hand, for a finite chain,

the sum over $n$ is not zero for any value of $\theta$ that allow an odd number of half-wavelengths to be present on the chain.

In terms of the electrical dipole moment operator associated with any vibrational mode, $\vec{p}_{\theta\ell}$, the interaction Hamiltonian can be written as

$$H_{int} = -\sum_{\theta,\ell} \vec{p}_{\theta\ell} \cdot \vec{E} \cos \Omega t. \tag{13}$$

Decomposing the dipole moment operator into its longitudinal and transverse components, it is readily seen that the longitudinal part is given by

$$p^L_{\theta\ell} = \sum_i e_i \left( \frac{\hbar N}{2m_i \omega_{\theta\ell}} \right)^{1/2} (\Delta_\theta q_{iz}(\theta, \ell)(a_{-\theta\ell} + a^\dagger_{\theta\ell}), \tag{14}$$

whereas the transverse part is given by

$$p^T_{\theta\ell} = \sum_i e_i \left( \frac{\hbar N}{2m_i \omega_{\theta\ell}} \right)^{1/2} (\Delta_{\theta-\psi} q^{(+)}_{i\ell\theta} + \Delta_{\theta+\psi} q^{(-)}_{i\ell\theta})(a_{-\theta\ell} + a^\dagger_{\theta\ell}). \tag{15}$$

To proceed with this analysis, we need to calculate the transition matrix element $H'_{if} \equiv < f|H_{int}|i >$, where $|i >$ and $|f >$ are the initial and final states of the system. In the most general case, we would consider the initial state of the system to be an equilibrium distribution of phonon states with $n_{\theta\ell}$ as the number of phonons (in the mode $\theta\ell$ in the state $|n_{\theta\ell} >$. If we consider one-phonon processes only, and further restrict our attention to the creation of one phonon (corresponding to the absorption of one photon), all we have to do is to replace the operator combination $a_{-\theta\ell} + a^\dagger_{\theta\ell}$ with $(n_{\theta\ell} + 1)^{1/2}$ in obtaining the matrix element. Thus the interaction matrix element can be decomposed into a longitudinal part

$$H'^L_{if} = -E_z \sum_i e_i \sum_{\theta,\ell} \left( \frac{\hbar N}{2m_i \omega_{\theta\ell}} \right)^{1/2} \Delta_\theta q_{iz}(\theta, \ell)(n_{\theta\ell} + 1)^{1/2}, \tag{16}$$

and a transverse part

$$H'^T_{if} = -E_t \sum_i e_i \sum_{\theta,\ell} \left( \frac{\hbar N}{2m_i \omega_{\theta\ell}} \right)^{1/2} (\Delta_{\theta-\psi} q^{(+)}_{i\ell\theta} + \Delta_{\theta+\psi} q^{(-)}_{i\ell\theta})(n_{-\theta\ell} + 1)^{1/2}. \tag{17}$$

The transition rate for the system to go from the $n$-phonon state to the $(n+1)$-phonon state in absorbing one incident photon is given by the Fermi golden rule,

$$\Gamma^{L,T} = \frac{2\pi}{\hbar} |H'^{L,T}_{if}|^2. \tag{18}$$

Table 1: Normal modes in the frequency region from 50 GHz to 350 GHz (data taken from Ref. 8)

| mode number | $\omega$ ($cm^{-1}$) | $\omega$ (GHz) | polarization | dipole moment (A.U.) |
|---|---|---|---|---|
| 1 | 2.92 | 87.6 | T | 0.003141 |
| 2 | 2.97 | 89.1 | L | 0.000288 |
| 3 | 3.67 | 110.1 | L | 0.000062 |
| 4 | 5.73 | 171.9 | L | 0.002209 |
| 5 | 7.72 | 231.6 | T | 0.000067 |
| 6 | 10.01 | 300.3 | T | 0.000154 |

The absorption coefficient is given by

$$\alpha^{L,T}(\Omega) = 2\hbar\Omega\Gamma^{L,T}/\epsilon_0 n^2 |E_{z,t}|^2. \tag{19}$$

Here $\epsilon_0$ is dielectric constant of free space and $n$ is the refractive index of the medium.

## 3.3 Sample Numerical Results

In this section we apply the formulation developed in the previous section to consider a typical case of absorption, obtaining some sample numerical results. These results will be compared with available experimental data.

In the frequency region of particular interest to us, from 50 GHz to about 350 GHz, Van Zandt et al have determined that there are six normal modes. Three of these are longitudinal and the other three are transverse. Table I lists some of the relevant physical quantities associated with these six modes.

Based on these data, we have evaluated the absorption coefficient, which is shown in Figure 5. In this calculation we have assigned an adjustable linewidth to each of the resonance

peaks. Such a linewidth has to be obtained from experimental data. Or alternatively, if the broadening mechanism is known, it can be calculated.

From the figure, it is seen that of the six modes predicted, only five are clearly visible. The first two (87.6 GHz and 89.1 GHz) are too close to be separated on this scale. The modes at 87.1 GHz has the largest dipole moment, followed by the one at 171.9 GHz. These are clearly reflected in the structure of the absorption spectrum. While the mode at 87.1 GHz gives rise to fairly sharp absorption feature, the one at 171.9 GHz is broad. The mode at 300.3 GHz is also distinguishable. However, the modes with the smallest dipole moments (110.1 GHz and 231.6 GHz) are only barely visible.

It should be pointed out that the original prediction of the normal modes is based on a model of DNA polymers in water solution. Some of the basic assumptions behind the predictions may not be valid in the case of dry DNA in aerosol samples. For example, without the surrounding water molecules (counterions) the vibrational frequencies are expected to shift higher (but there is no reason to expect that the number of normal modes should change); Secondly, in the dry samples the polymers are more likely to be folded, and otherwise oriented randomly; A third difference is that in the dry samples the polymers are in very proximity of one another, and it is likely that inter-chain interactions have to be considered.

Thus it is reasonable to expect that the above calculation and only serve as a guide in interpreting data from thin films, powders, and aerosols in the sense that although the number of modes should be the same, they may not be at the same frequencies as in the case of aqueous solutions. To be more specific, we expect that the frequencies should be shifted higher in the dry samples. Intuitively one would expect this: the surrounding counterions represent additional friction or viscosity, which serve to impede the vibrational motion of the atoms on the DNA polymer chain.

We have recently measured the absorption spectrum of DNA samples of thin films and powders in the frequency region of 180 GHz - 220 GHz [18]. All the samples show 2 or 3 broad absorption features in this spectral region. It is tempting to try to identify these with some of the predicted vibrational modes. The most likely candidates would be the four lower modes ( 87.6 GHz, 89.1 GHz, 110.1 GHz, 171.9 GHz), shifted to higher frequencies.

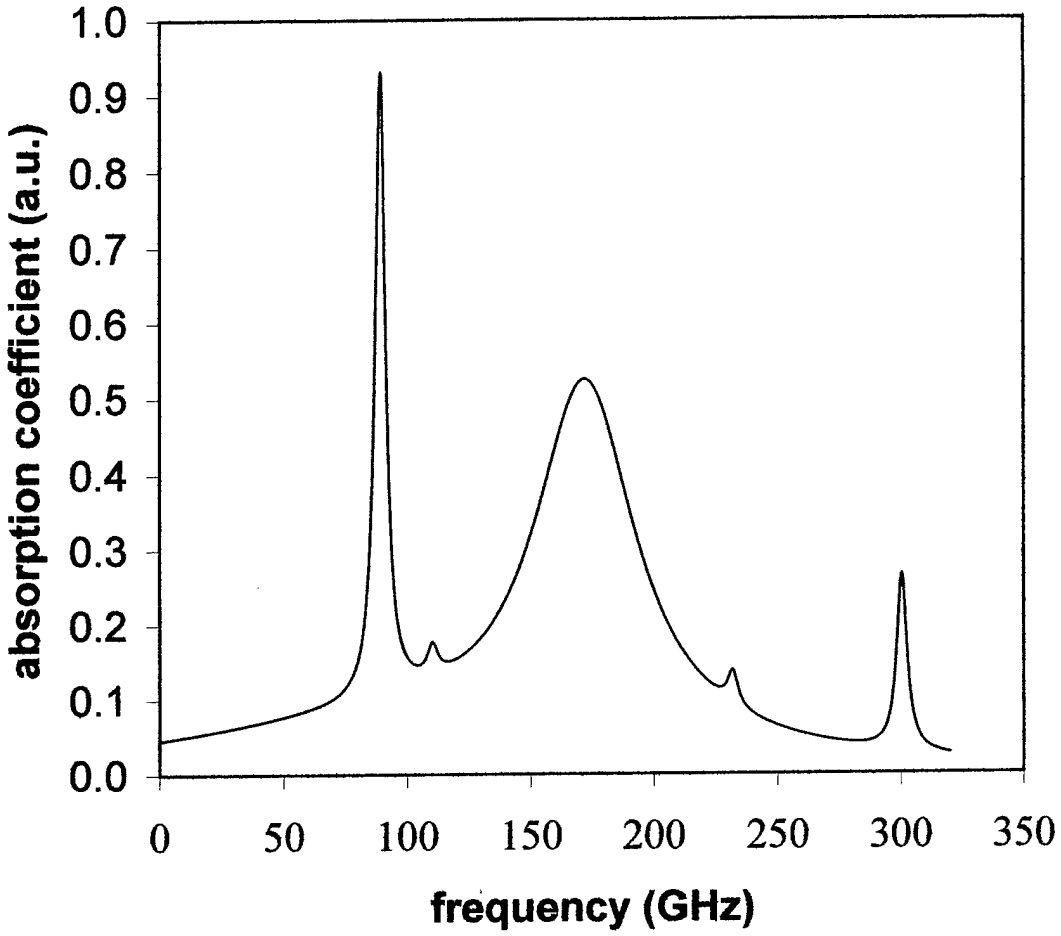


Figure 5: Absorption spectrum in the microwave/millimeter wave region by a long chain DNA polymer.

However, further, more definitive identifications can only be made with more refined data. which we are in the process of obtaining by using aerosol samples.

# 4 Summary

To summarize, we have developed an experimental technique to measure the millimeter wave absorption spectrum of DNA polymers. Several aerosol samples were measured and the results are very promising. We are currently refining the experimental technique to achieve better resolution. We have also developed a formalism of calculation of microwave/millimeter wave absorption coefficient of DNA polymers. This formalism relies on a normal mode analysis of the DNA polymer system to provide the eigenmode frequencies and associated eigenvectors. The latter information, along with the atomic partial charge data, is used to calculate the dipole moment corresponding to each normal mode. The quantum mechanical transition matrix elements are evaluated with the dipole moment operators and phonon occupation-number states. The transition rate and the absorption coefficient are then evaluated. We have applied the theory to study the absorption of electromagnetic radiation in the frequency region of 50 GHz to 350 GHz, using available theoretical predictions on the normal modes. The theoretical results are compared with recent experimental studies of millimeter wave absorption in this spectral region.

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